MRT Methodologies for Application to Nuclear Safeguards, Safety and Security

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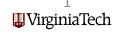
Virginia Tech Transport Theory Group (VT³G)

Director of Nuclear Engineering and Science Lab (NSEL) at Arlington Nuclear Engineering Program, Mechanical Engineering Department



Energy Seminar Series





Nuclear Science and Engineering Lab (NSEL) @ Arlington

NSEL at Arlington Operates under auspices of ICTAS* and Mechanical Engineering Department. It engages with various entities/organizations at Virginia Tech and beyond to address different applications including power, security, medicine, and policy (http://nsel.ncr.vt.edu)



Collaborations @ Virginia Tech

Virginia Tech	Activity	Campus		
Physics Department	Neutrino Physics Center, GEM*STAR initiative	Blacksburg		
Nuclear Engineering Program	Education & research	Blacksburg		
Discovery Analytics Center	Inference and detection	NCR		
Hume Center for national security	Cyber security	NCR		
School of Public and International Affairs (SPIA) & Department of Science and Technology in Society	Nuclear nonproliferation and policy	NCR		



^{*}Institute of Critical Technology and Applied Science

Collaborations with other organizations

Organization	Activity	Location		
US Naval Academy (USNA)	 S Naval Academy (USNA) Signed a research and education partnership, Aug 2015 Initiated benchmarking of the RAPID code system using USNA's subcritical facility (for nuclear safeguards) Discussing establishing a special graduate program for USNA graduates 			
Naval Surface Warfare Center, Carderock	Tandem linear accelerator research; small modular reactor use in military	MD		
Federation of American Scientist	Workforce on LEU nuclear fueled naval vessels	DC		
Georgia Tech (lead) with 10 other organizations including VT	Design of Integral Inherently Safe LWR reactor system design	Company - Georgia Tectr - Mr Maretinge.		
George Washington University	Nuclear education; GEM*STAR	I2SDEWR		
Oak Ridge National Lab	GEM*STAR, spent fuel casks	Tennessee		
Collaboration among NE, Physics & MSE	Safe, Secure, Sustainable Nuclear Power (S3NPower)	Blacksburg, ICTAS		





http://www.virginianuclear.org/

Formation of VNEC nonprofit organization									
Organization	Activities	Location							
Virginia Nuclear Energy Consortium (VNEC)	 Promotion of nuclear industry, education and research 	Virginia							
	 Membership include: AREVA, B&W, Dominion, GE, Newport News Shipbuilding, UVA, VCU, and VT 								
	 Prof. Haghighat is Chairman of the Board 								

NSEL – Organization of Workshops/Forums

Year (date)	Title
2011 (Nov 7-11)	13 th International Workshop on Particle Transport Simulation of Nuclear Systems (http://www.cpe.vt.edu/transport)
2012 (March 11-12)	Symposium on Low Power Critical Facilities (LPCF) in collaboration with SUNRISE* (http://www.cpe.vt.edu/lpcf)
2012 (Nov 5)	Forum on Nuclear Regimes: Future Outlooks; sponsors included AREVA, ICTAS, VT-NCR, and partners included Naval Postgraduate school, Federation of American Scientists, and George Washington's Elliot College of International Affairs (http://www.ictas.vt.edu/nuclear)
2013 (Aug 7)	Seminar on nuclear power & education for a group of international reporters (at the request of Department of State) (http://nsel.ncr.vt.edu)
2014 (July 20)	a half-day workshop on "Advanced particle transport methodologies/tools for nuclear safeguards and non-proliferation," INMM 55 th Annual Meeting, Atlanta, Georgia. (In collaboration with Georgia Tech)
2014 (Sept 28)	A half-day workshop on "Hybrid particle transport methods for solving complex problems in real-time," PHYSOR 2014 International Conference, Kyoto, Japan. (In collaboration with Georgia Tech)
2014 (Dec 15-18)	MRT Methodologies for Real-Time Simulation of Nuclear Safeguards & Nonproliferation Problems,' Modeling and Simulation for Safeguards and Nonproliferation <i>Workshop ORNL</i> .
2015 (June 23-25)	1 st Workshop on Methodologies for Spent Nuclear Fuel Pool Simulations (Safety and Safeguards) (http://www.cpe.vt.edu/nuclear)

^{*}Southeast Universities Nuclear Reactors Institute for Science and Education

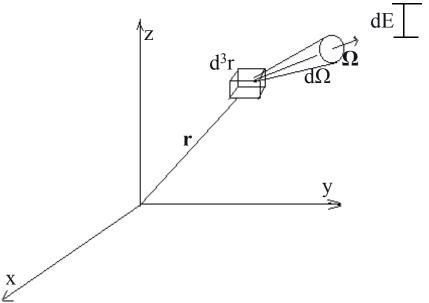


Particle Transport Theory

Objective

Determine the expected number of particles in a phase space ($d^3rdEd\Omega$) at time t:

$$n(\vec{r}, E, \hat{\Omega}, t)d^3rdEd\Omega$$



Number density is used to determine <u>angular flux/current</u>, <u>scalar flux and current</u> <u>density</u>, <u>partial currents</u>, <u>and reaction rates</u>.



Simulation Approaches

Deterministic Methods

 Solve the linear Boltzmann equation to obtain the expected flux in a phase space

Statistical Monte Carlo Methods

 Perform particle transport <u>experiments</u> using random numbers (RN's) on a computer to estimate average properties of a particle in phase space



Deterministic – Linear Boltzmann Equation

• Integro-differential form

streaming collision $\hat{\Omega}.\nabla\Psi(\vec{r},E,\hat{\Omega}) + \sigma(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega}) = \text{scattering}$ $\int_{0}^{\infty} dE' \int_{4\pi} d\Omega' \sigma_{s}(\vec{r},E' \to E,\hat{\Omega}' \to \hat{\Omega})\Psi(\vec{r},E',\hat{\Omega}) + \text{Independent source}$ $\frac{\chi(E)}{4\pi} \int_{0}^{\infty} dE' \int_{4\pi} d\Omega' \upsilon \sigma_{f}(\vec{r},E')\Psi(\vec{r},E',\hat{\Omega}) + S(\vec{r},E,\hat{\Omega})$

Integral form

$$\psi(\vec{r}, E, \hat{\Omega}) = \int_{0}^{R} d |\vec{r} - \vec{r'}| Q(r') e^{-\tau_{E}(\vec{r}, \vec{r'})} + \psi(\vec{r}_{s}, E, \hat{\Omega}) e^{-\tau_{E}(\vec{r}, \vec{r'})}$$

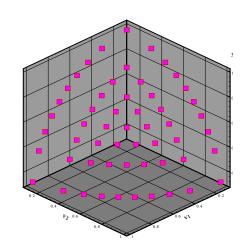


Integro-differential - Solution Method

• Angular variable: Discrete Ordinates (Sn) method:

A discrete set of directions $\{ \hat{\Omega}_m \}$ and associated weights $\{ \mathbf{w_m} \}$ are selected

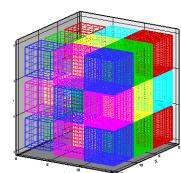
$$\hat{\Omega}_{m}.\nabla\Psi(\vec{r},E,\hat{\Omega}_{m}) + \sigma(\vec{r},E)\Psi(\vec{r},E,\hat{\Omega}_{m}) = q(\vec{r},E,\hat{\Omega}_{m})$$



Spatial variable

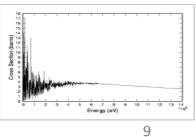
Integrated over <u>fine meshes</u> using FD or FE methods

$$\Psi_{m,g,A} = \frac{\int d^3 r \Psi_{m,g}(\vec{r})}{\Delta V_{ijk}}$$



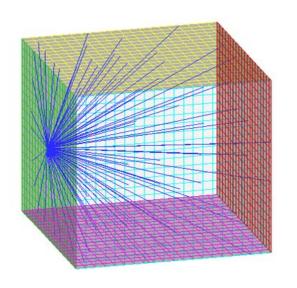
Energy variable

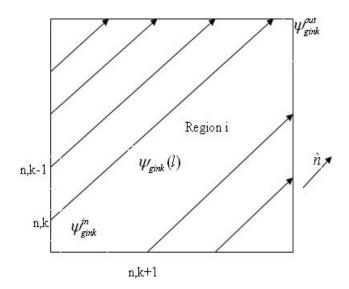
Integrate over energy intervals to prepare multigroup cross sections, $\sigma_{\!\scriptscriptstyle g}$



Integral - Solution method

Method of Characteristic (MOC): Model is partitioned into coarse meshes and transport equation is solved along the characteristic paths (k) (parallel to each discrete ordinate (n)), filling the mesh, and averaged





$$\psi_{g,m,i,k}(t_{m,i,k}) = \psi_{g,m,i,k}(0) \exp(-\sigma_{g,i}t_{m,i,k}) + \frac{Q_{g,m,i}}{\sigma_{g,i}}(1 - \exp(-\sigma_{g,i}t_{m,i,k}))$$



Deterministic - Issues/Challenges/Needs

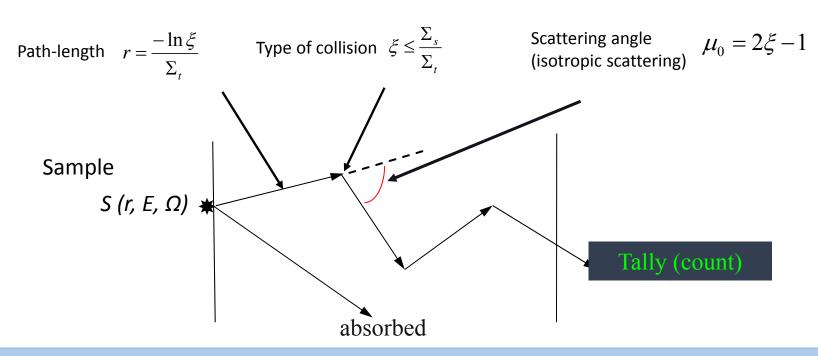
- Robust <u>numerical</u> formulations (e.g., adaptive differencing strategy)
- Algorithms for improving <u>efficiency</u> (i.e., acceleration techniques
 synthetic formulations and pre-conditioners)
- Use of advanced computing <u>hardware & software</u> environments
- Pre- and post-processing tools
- > Multigroup cross section preparation
- > Benchmarking

Over the past 29 years, VT³G address all the above issues



Monte Carlo Methods

 Perform an experiment on a computer; "exact" simulation of a physical process



<u>Issues</u>

- Precise expected values; i.e., small relative uncertainty, $R_{\bar{x}} = \frac{\sigma_{\bar{x}}}{\bar{x}}$, requiring large computation time
- > Therefore, Variance Reduction techniques are needed for real-world problems!
- > For eigenvalue problems, the source convergence is an added difficulty.



Deterministic vs. Monte Carlo

Item	Deterministic	MC
Geometry	Discrete/ Exact	Exact
Energy treatment – cross section	Discrete	Exact
Direction	Discrete/ Truncated series	Exact
Input preparation	Difficult	simple
Computer memory	Large	Small
Computer time	Small	Large
Numerical issues	Convergence	Statistical uncertainty
Amount of information	Large	Limited
Parallel computing	Complex	Trivial



Why not MC only?

- Because of the difficulty in obtaining detail information with reliable statistical uncertainty in a reasonable time; examples are:
 - Real-time simulations
 - Obtaining energy-dependent flux distributions,
 - Time-dependent simulations,
 - Sensitivity analysis,
 - Determination of uncertainties



Why not use advanced hardware?

- ➤ VT³G has developed vector and parallel algorithms:
 - Developed two large codes: PENTRAN (1996) and TITAN (2004)

Why not use hybrid methods?

- Deterministic-deterministic (differencing schemes, different numerical formulations, generation of multigroup cross sections, generation of angular quadratures, acceleration techniques)
 - VT³G has developed various algorithms; a few have been implemented in PENTRAN and TITAN
- Monte Carlo-deterministic (variance reduction with the of use deterministic adjoint)
 - VT³G has developed CADIS, A³MCNP in 1997; CADIS has become popular recently!



Remarks

 Particle transport-based methodologies are need for real-time simulation

 Even 'Fast' particle transport codes, with parallel and hybrid algorithms, are slow because of large number of unknowns



Development of Transport Formulations for Real-Time Applications

- Physics-Based transport methodologies are needed:
- Developed Multi-stage, Response-function Transport (MRT) methodology
 - Based on problem physics partition a problem into stages (subproblems),
 - For each stage employ response method and/or adjoint function methodology
 - Pre-calculate response-function or adjoint-function using an accurate and fast transport code
 - Solve a linear system of equations to couple all the stages



Examples for MRT Algorithms

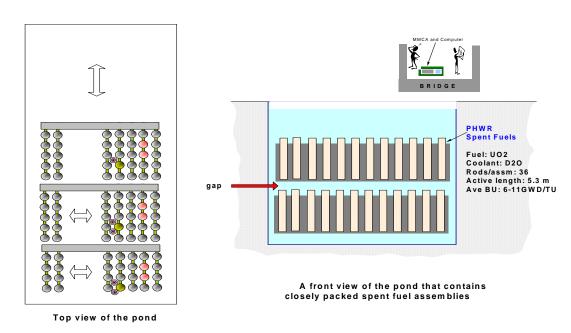
- Nondestructive testing: Optimization of the Westinghouse's PGNNA active interrogation system for detection of RCRA (Resource Conversation and Recovery Act) (e.g., lead, mercury, cadmium) in waste drums (partial implementation of MRT; 1999)
- Nuclear Safeguards: Monitoring of spent fuel pools for detection of fuel diversion (2007) (funded by LLNL)
- **Nuclear nonproliferation:** Active interrogation of cargo containers for simulation of special nuclear materials (SNMs) (2013) (in collaboration with GaTech)
- **Spent fuel safety and security:** Real-time simulation of spent fuel pools for determination of eigenvalue, subcritical multiplication, and material identification (partly funded by I²S project, led by GaTech) (Ongoing)
- Image reconstruction for SPECT (Single Photon Emission Computed
 Tomography): Real-time simulation of an SPECT device for generation of project
 images using an MRT methodology and Maximum Likelihood Estimation
 Maximization (MLEM) (filed for a patent, June 2015)



Nuclear Safeguards - Inspection of spent nuclear fuel pool

- Goal: Develop accurate and fast hybrid methodology and tool for inspection of spent fuel pool; funded by LLNL
- Approach: Use measurement and <u>on-line</u> computation to obtain trending curves

Atucha-1 Spent fuel pool





Issues

- Develop a fast and accurate computation tool which can estimate the detector response for various combinations of
 - **>** Burnup
 - ➤ Cooling time
 - ➤ Pool lattice arrangement
 - > Fuel type (enrichment)



MRT Methodology

Online Calculation of <u>detector response</u> (R):

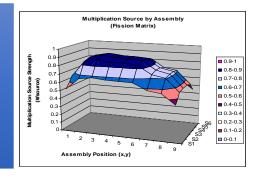
Neutron source

$$R_n = \langle S_n \phi_n^+ \rangle$$

Adjoint (Importance) function

- Source (S = S_{intrinsic} + S_{subcritical-Multiplication})
 - Stage 1 Intrinsic Source
 - Spontaneous fission & (α, n) from fuel burnup calculation (ORIGEN-ARP)

(Created a database)

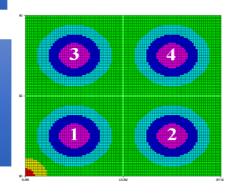


- Stage 2 Subcritical Multiplication (Hybrid method)
 - Simplified fission-matrix (FM) method
 - Use MCNP Monte Carlo to obtain $a_{i,j}$ for each pool type

(Created a database for coef. a_{ii})

$$F_i = \sum_{i=1}^{N} a_{i,j} (F_j + S_j^{\text{int.}})$$

- Adjoint function
 - Stage 3 Is obtained using the PENTRAN transport code (Created a database for multigroup adjoint for different lattice sizes)



Adjoint Function Methodology

"Forward" Transport Equation

$$H \psi = q$$
 in V
$$\psi = 0$$
 on Γ for $\hat{n} \cdot \hat{\Omega} < 0$

where

$$H = \hat{\Omega} \cdot \nabla + \sigma_t(\vec{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, E' \to E, \hat{\Omega}' \to \hat{\Omega})$$

"Adjoint" Transport Equation

$$H^+\psi^+ = q^+ \quad \text{in V}$$

$$\psi^+ = 0 \quad \text{on } \Gamma \text{ for } \hat{n} \cdot \hat{\Omega} > 0$$

where

$$H^{+} = -\hat{\Omega} \cdot \nabla + \sigma_{t}(\vec{r}, E) - \int_{0}^{\infty} dE' \int_{4\pi} d\Omega' \sigma_{s}(\vec{r}, E \to E', \hat{\Omega} \to \hat{\Omega}')$$



Adjoint function methodology – Detector response

Forward approach
$$R = \langle \sigma_d \psi \rangle = \int_{V_d} dV \int_0^\infty dE \int_{4\pi} d\Omega \ \sigma_d(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega})$$

 The "commutation relation" between the "forward" and "adjoint" transport equations

$$\left\langle \psi^{+} H \psi \right\rangle - \left\langle \psi H^{+} \psi^{+} \right\rangle = \left\langle \psi^{+} q \right\rangle - \left\langle \psi q^{+} \right\rangle$$

Then,

$$\left\langle \psi q^{\scriptscriptstyle +} \right\rangle = \left\langle \psi^{\scriptscriptstyle +} q \right\rangle$$

• If we consider $q^+ = \sigma_d$

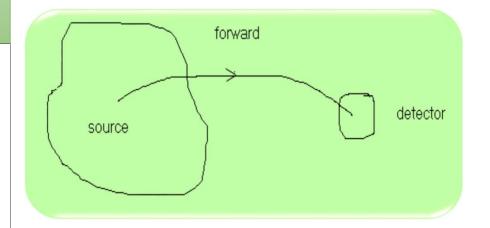
$$R = \left\langle \psi^+ \, q \right\rangle$$



Demonstration

Standard

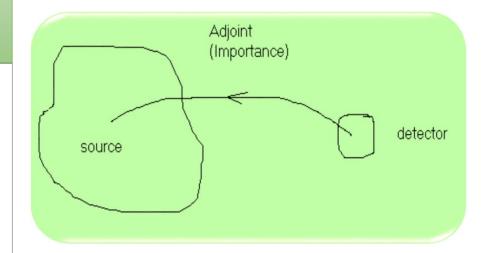
$$R = <\sigma_d \phi >$$
 Where, $H\phi = S$



Adjoint Methodology

$$R = \langle S\phi^+ \rangle$$

Where,
$$H^{\scriptscriptstyle +}\phi^{\scriptscriptstyle +}=\sigma_d^{}$$



Derivation of Fission Matrix (FM) Formulation

Eigenvalue formulation in operator form is expressed by

$$H\psi(\bar{p}) = \frac{1}{k}F\psi(\bar{p})$$

Where,

$$\begin{split} \bar{p} &= (\bar{r}, E, \widehat{\Omega}) \\ H &= \widehat{\Omega} \cdot \nabla + \sigma_t(\bar{r}, E) - \int_0^\infty dE' \int_{4\pi} d\Omega' \, \sigma_s(\bar{r}, E' \to E, \mu_0) \end{split}$$

$$F = \frac{\chi(E)}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \, \nu \sigma_f(\bar{r}, E')$$

FM Derivation (cont)

We may rewrite above equation as

$$S(\bar{p}) = \frac{1}{k} A S(\bar{p})$$

Where,

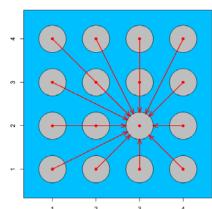
$$S = \tilde{F}\psi$$
, $A = \tilde{F}H^{-1}\chi$, & $\tilde{F} = \frac{1}{4\pi} \int_0^\infty dE' \int_{4\pi} d\Omega' \nu \sigma_f(\bar{r}, E')$



Fission Matrix (FM) Formulation

Eigenvalue

$$F_i = \frac{1}{k} \sum_{j=1}^{N} a_{i,j} F_j$$



- *k* is eigenvalue
- F_i is fission source, S_i is fixed source in cell j
- $a_{i,j}$ is the number of fission neutrons produced in cell *i* due to a fission neutron porn in cent *j*.

• Subcritical multiplication

$$F_i = \sum_{j=1}^{N} (a_{i,j}F_j + b_{i,j}S_j^{Intrinsic}),$$

$$M = \frac{\sum_{j=1}^{N} (F_j + S_j^{intrinsic})}{\sum_{j=1}^{N} S_j^{intrinsic}}$$

• $b_{i,j}$ is the number of fission neutrons produced in cell i due to a source neutron born in cell j.

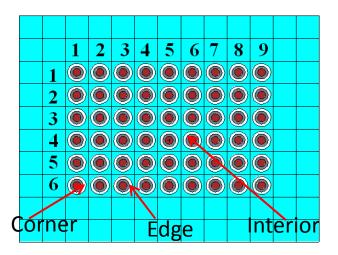


Fission Matrix Coefficients – Inspection of Pool

• For this safeguards application, we have demonstrated that within the expected tolerance, the $b_{i,j}$ coefficients are equivalent to $a_{i,j}$, therefore, subcritical multiplication fission density is expressed by

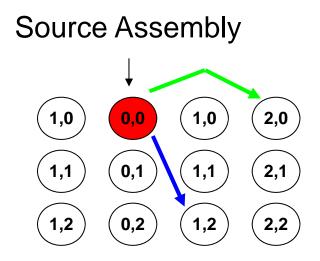
$$F_{i} = \sum_{i=1}^{N} a_{i,j} (F_{j} + S_{j})$$

• Further, we have demonstrated that again within the tolerance, we need only three sets of coefficients depending on the position of assemblies, i.e., corner, edge, and interior





Calculation of FM coefficients



Fission Matrix Coefficients									
	x-distance from source assembly								
y-distance	0 1 2								
0	2.13E-01	4.98E-02	2.70E-03						
1	4.56E-02	1.38E-02	1.22E-03						
2	2.18E-03	1.11E-03							

Coefficients for corner, edge and interior assemblies are within 1%

Hence, this finding reduces the necessary calculations to only one assembly location for different burnups and cooling time



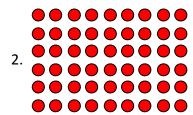
Testing the Simplified FM Methodology

Four test spent fuel scenarios

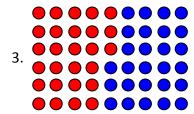
• 2x6 array, uniform source

1.

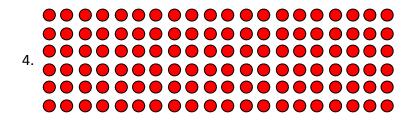
9x6 array, uniform source



 9x6 array, 27 assemblies on the left with source strength 1, the rest with source strength 0.5



• 20x6 array, uniform source



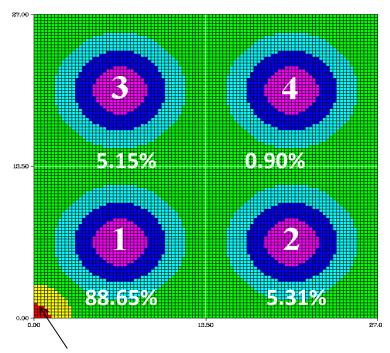
FM Testing Results

- Excellent agreement with Monte Carlo (<1%)
- Very fast
 - <1s for Fission-matrix method
 - ~1hr for Monte Carlo

Assembly Arrangement Case	M (MCNP)	M (Fission Matrix)	Difference	MCNP Uncertainty 1-σ
2x6, uniform	1.7133	1.7104	-0. 29%	8000.0
9x6, uniform	1.9988	1.9966	-0. 22%	0.0007
9x6, non-uniform	2.0033	1.9968	-0.65%	0.0013
20x6, uniform	2.0513	2.0444	-0. 69%	0.0012

Detector FOV

$$FR_i = \frac{\sum_{g} \psi_{ig}^* S_{ig} V_i}{\sum_{j} \sum_{g} \psi_{jg}^* S_{jg} V_j}$$



Fission Chamber (94 w% U-235)



INSPCT-S

(Inspection of Nuclear Spent fuel-Pool Computing Tool —Spreadsheet)

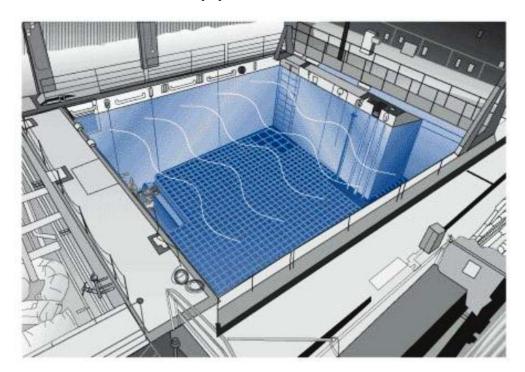
INSPCT-S solves

$$R_n = \langle S_n \phi_n^+ \rangle$$

PUT										OUTPUT									
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3	11000	11000	11000	11000	11000	11000	11000	11000		3	1.00E+08	8.04E+07	6.86E+07	5.84E+07	5.06E+07	4.29E+07	3.23E+07	25047256	
4	12000	12000	12000	12000	12000	12000	12000	12000		4	1.42E+08	1.17E+08	1.01E+08	8.51E+07	7.33E+07	6.15E+07	4.53E+07	34204842	
5	13000	13000	13000	13000	13000	13000	13000	13000		5	1.98E+08	1.67E+08	1.45E+08	1.22E+08	1.04E+08	8.67E+07	6.28E+07	46492994	
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6.5										6.5	0.57336	1.093457							
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										0.5									
										1.5		3.36%				-15.25%			
										2.5				3.82%					
										3.5									
										4.5				-3.65%					
										5.5						4.74%			
										6.5									
																			2.4

Real-time simulations of commercial spent fuel pools

Criticality Safety, Nonproliferation & Safeguards applications





Background

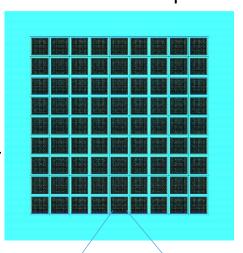
- Standard approach Full Monte Carlo calculations face difficulties in this area
 - Convergence is difficult due to low coupling between regions (due to absorbers)
 - Convergence can also be difficult to detect
 - Computation times are very long, especially to get detailed information
 - Changing pool configuration requires complete recalculation
- Fission Matrix (FM) approach It can address the above issues
 - Fission matrix coefficients are pre-calculated using Monte Carlo
 - Computation times are much shorter, with no convergence issues
 - Detailed fission distributions are obtained at pin level
 - Changing pool assembly configuration does not require new precalculations (No additional Monte Carlo)

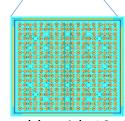


Developed a Multi-stage methodology for determination of FM coefficients

- As the computational size (for I²S reactor design)
 - $N = 9 \times 9 \times 336 = 27,216$ total fuel pins/ fission matrix cells
 - Considering 24 axial segments per rod, then
 - N = 653,184
- Standard FM would require N = 653,184 separate fixed-source calculations to determine the coefficient matrix
 - A matrix of size N x N = 4.26649E+11 total coefficients (> 3.4 TB of memory is needed)
- The standard approach is clearly NOT feasible
- We have developed a multi-stage approach to obtain detailed FM coefficients (in the process of filing for a patent)

9x9 array of assemblies in a pool





Assembly with 19x19 lattice; 25 positions are reserved for control rods



RAPID tool

- Developed the RAPID (Real-time Analysis spent fuel Pool *In situ* Detection) tool for determination of
 - Eigenvalue
 - Subcritical multiplication
 - Pin-wise, axially-depdendent fission density
- With application to
 - Criticality safety
 - Safeguards
 - Nonproliferation and materials accountability



RAPID code system - Structure

Pre-Calculation (one time):

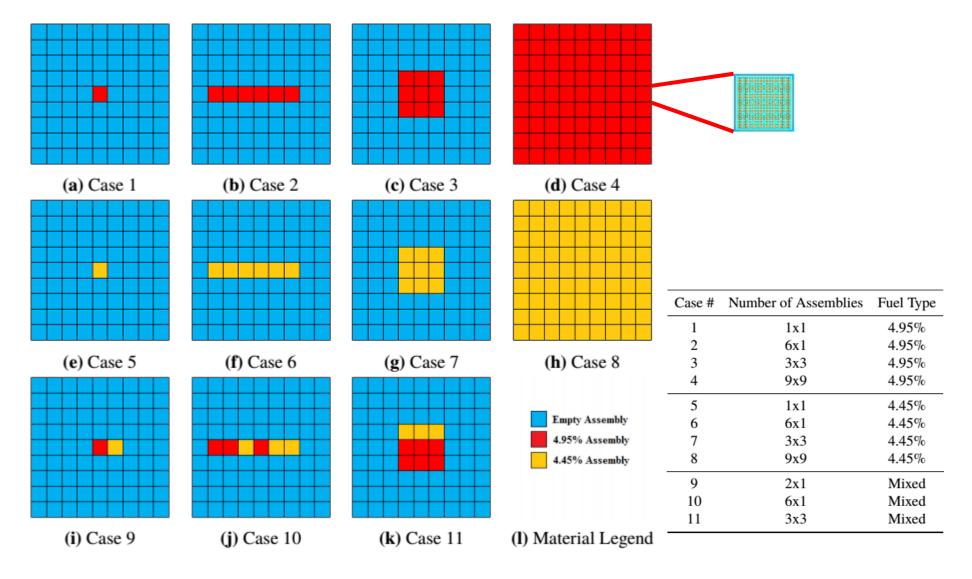
- 1. Burnup Calculation to obtain material composition
- 2. Fission Matrix Coefficient Generation

Real-time Analysis:

- 1. Run Fission Matrix Code
- 2. Process Results

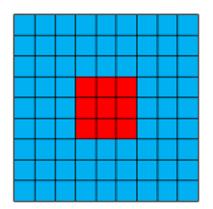


Test Problems (9x9 assemblies)





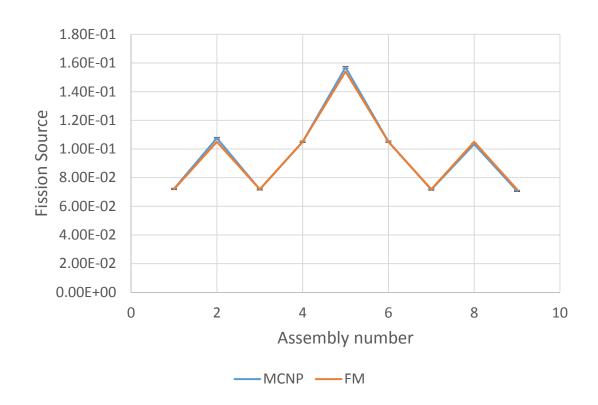
Case 3 Eigenfunction



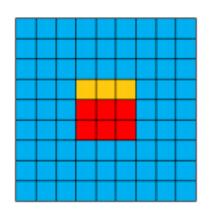
Reference Solution



Comparison of RAPID with MC



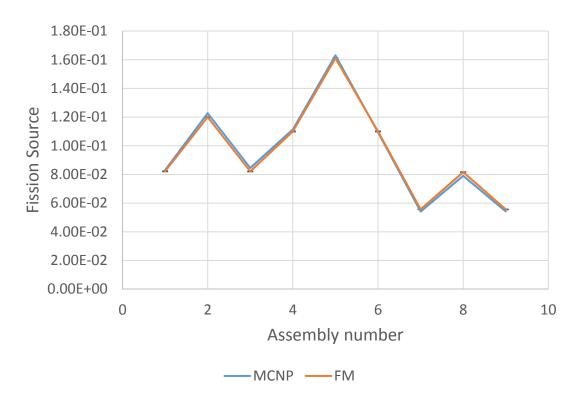
Case 11 Eigenfunction



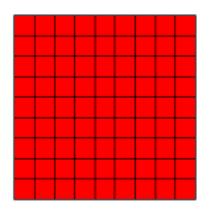
Reference Solution



Comparison with RAPID with MC



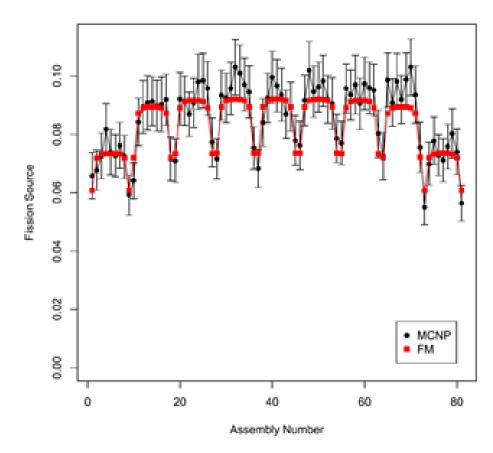
Case 4 Eigenfunction distribution



Reference Solution



Comparison with RAPID with MC



Comparison of calculated M - RAPID vs. MCNP

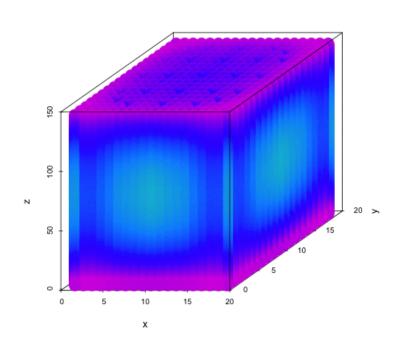
Case	FIV	1		MCNF		Error in M	Speedup
	M	Time (min)	M	Time (min)	1-σ Uncertainty	(FM vs MCNP)	(FM vs MCNP)*
1x1	3.343353	0.092	3.33155	925	0.0010	0.35%	10062
6x1	4.328244	0.213	4.31336	1198	0.0010	0.35%	5613
3x3	5.428051	0.965	5.40992	1502	0.0011	0.35%	1558
9x9	6.697940	8.17	6.67674	1928	0.012	0.32%	236

^{*}Note that the *RAPID* also provide pin-wise, axial-dependent fission source or power.

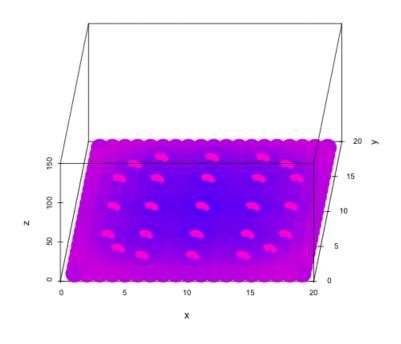


3-D Fission Density

Y-LEVEL ANIMATION



Z-LEVEL ANIMATION





Conclusion

MRT methodology allows for development of real-time tools for analysis of nuclear systems



Thanks!

Questions?

Monte Carlo Methods for Particle Transport Alireza Haghighat CRC Press

